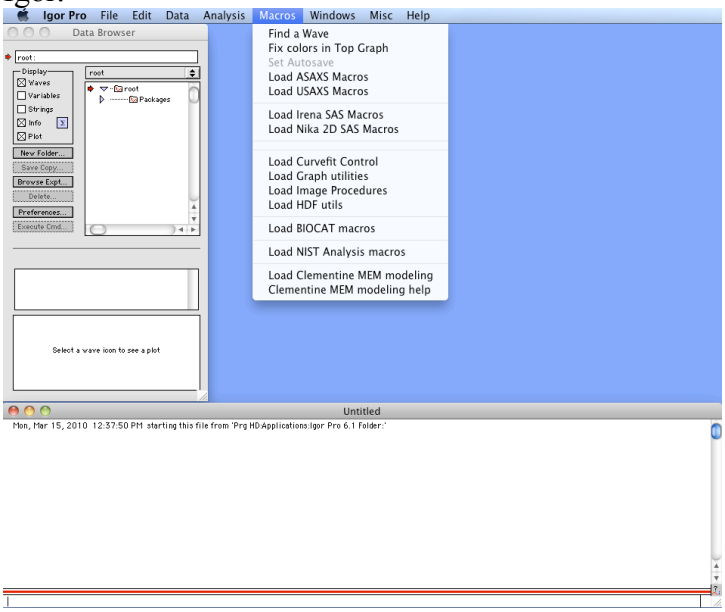
Modeling II tool in Irena package

This handout describes how SAS data (example using provided data from USAXS instrument) can be fitted using Modeling II tool in Irena using two log-normal size distribution of spheres. Test data provided were measured in 2001 and represent SAS from samples of alumina polishing powders. The powders were spread on sticky tape and covered with another layer of the same tape (sticky sides towards each other). Same two tapes were subtracted as empty run. The data are not, however, calibrated as the sample thickness of these samples is not really meaningful.

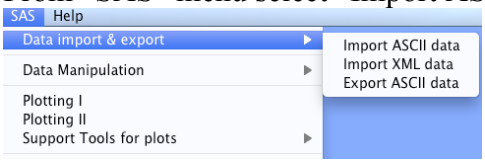
Start Igor, load macros

Start Igor Pro, from the menu "Macros" select the "Load Irena SAS Macros". This will add new menu SAS in Igor.

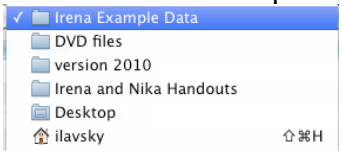


Import data

From "SAS" menu select "Import ASCII data".

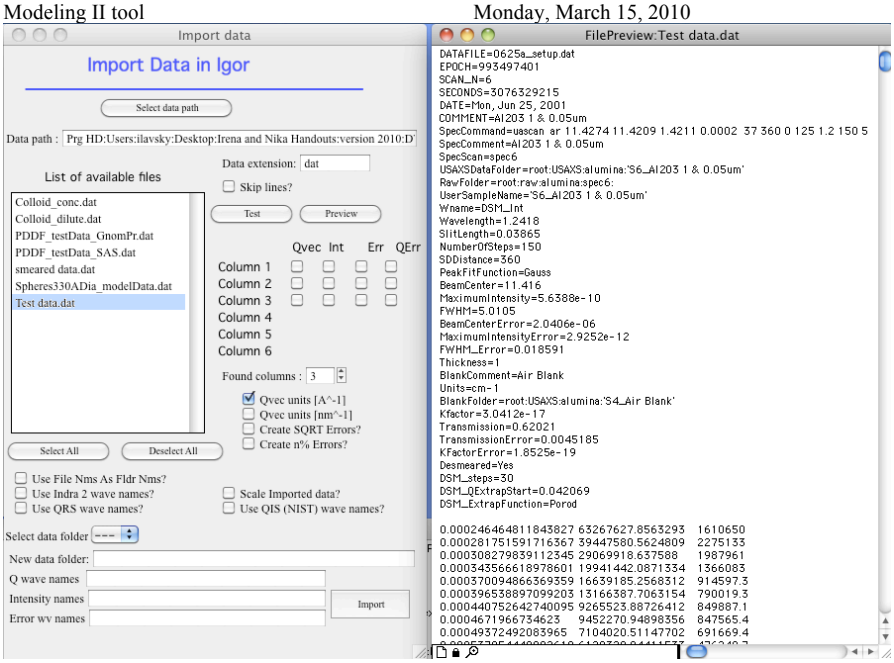


This will create new panel. Push the button "Select data path" and navigate to folder, where are the data.

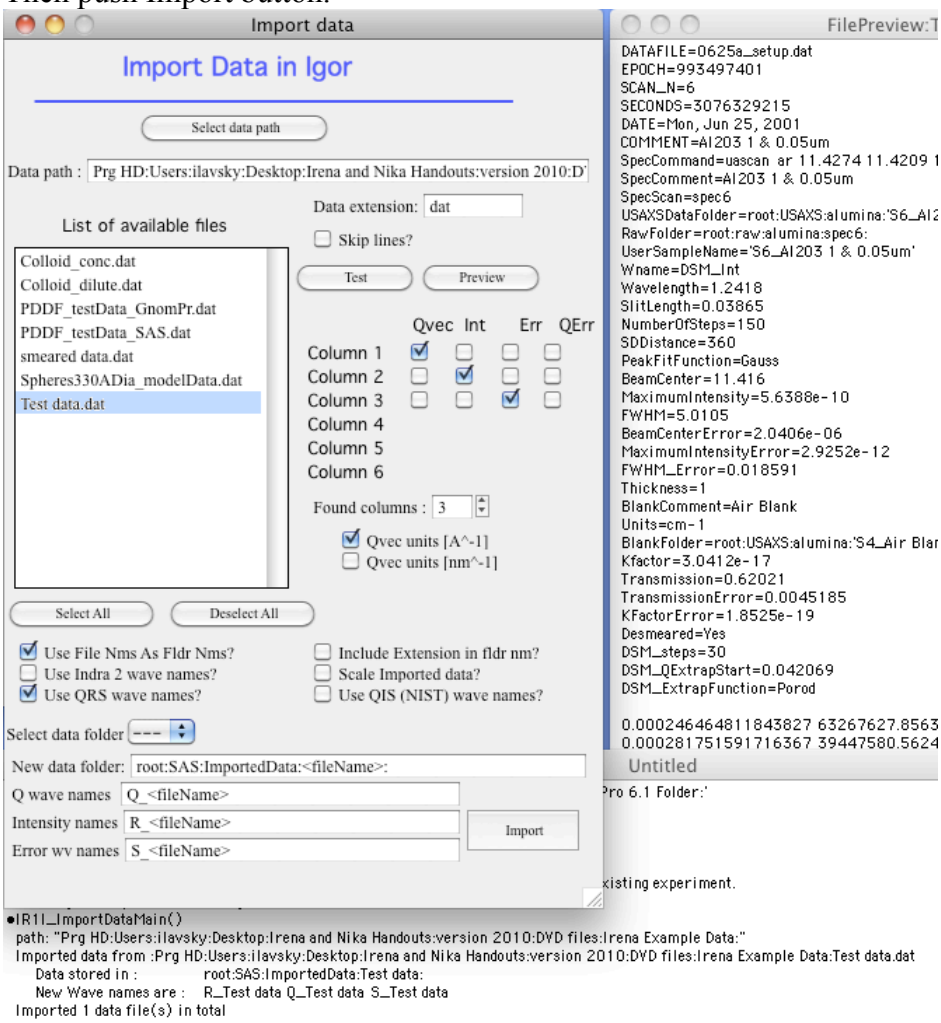


The test data provided (Test data.dat) have extension dat, we can put this in the "Data extension" field and only files with this extension will show.

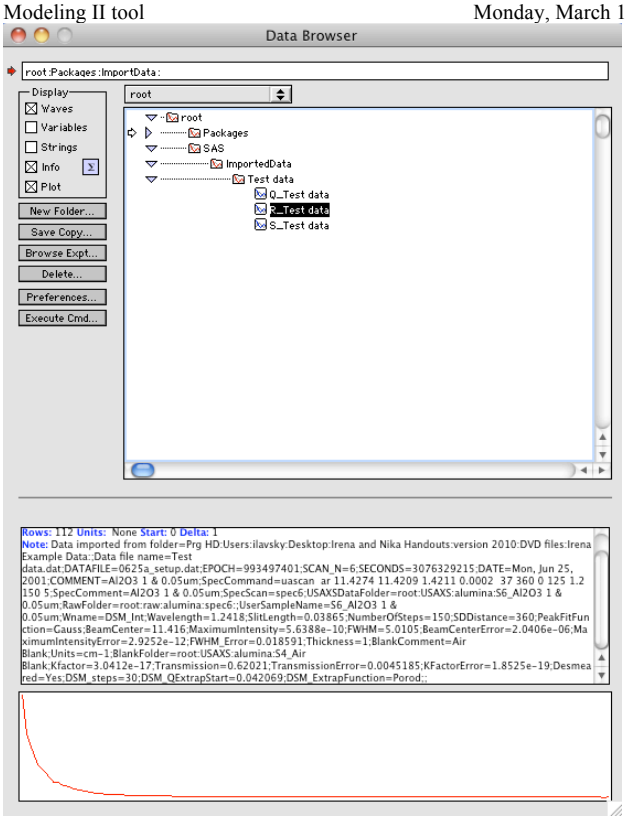
Select the "Test data.dat" and push buttons "test" and "Preview". The Test will find how many columns of data are in the file and Preview will open this file for our previews in separate window.



Note, that after header this files contains 3 columns – q, intensity and error estimates. Close preview and check the checkbox for column 1 as Qvec, column 2 as Int and column 3 as Err.
Select "Use File Nms as Fldr Nams?" and "Use QRS wave names". Select the file with data (Test data.dat). Then push Import button.



This will import the data into Igor – see below:

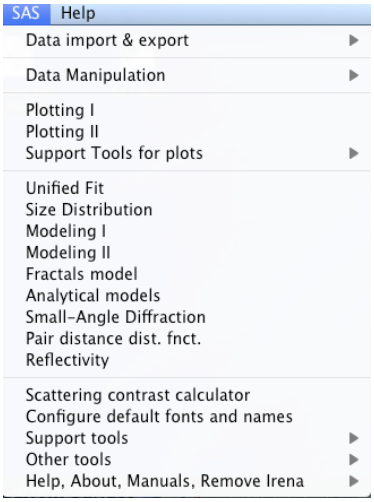


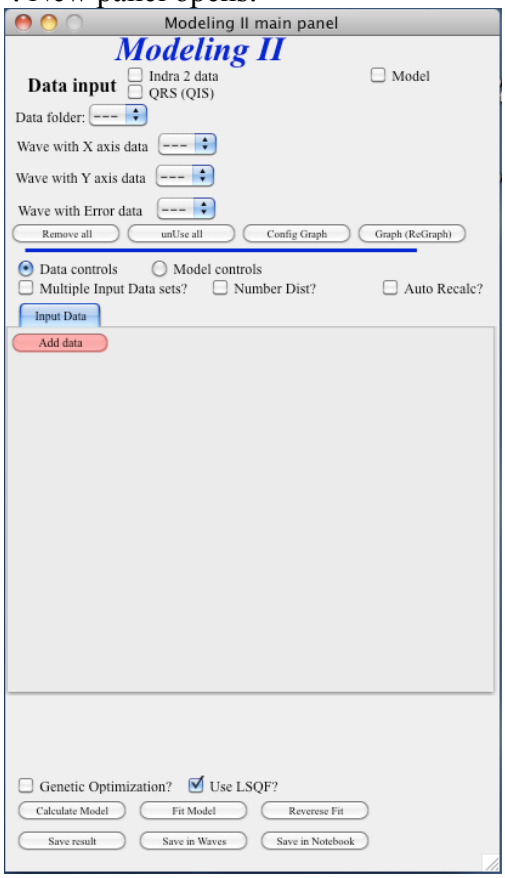
Just for information: Note, that the header from the ASCII file we had is now attached to the wave in so called wavenote – it is visible, when you select the wave in the Data browser and have the "info" checkbox checked. This is how Irena macros store additional information with waves – as wavenotes, which are text files attached to the waves.

Using Modeling II tool

Setup

Close all import-related windows (Panel and Notebook).
Select from SAS Menu “Modeling II”. New panel opens:





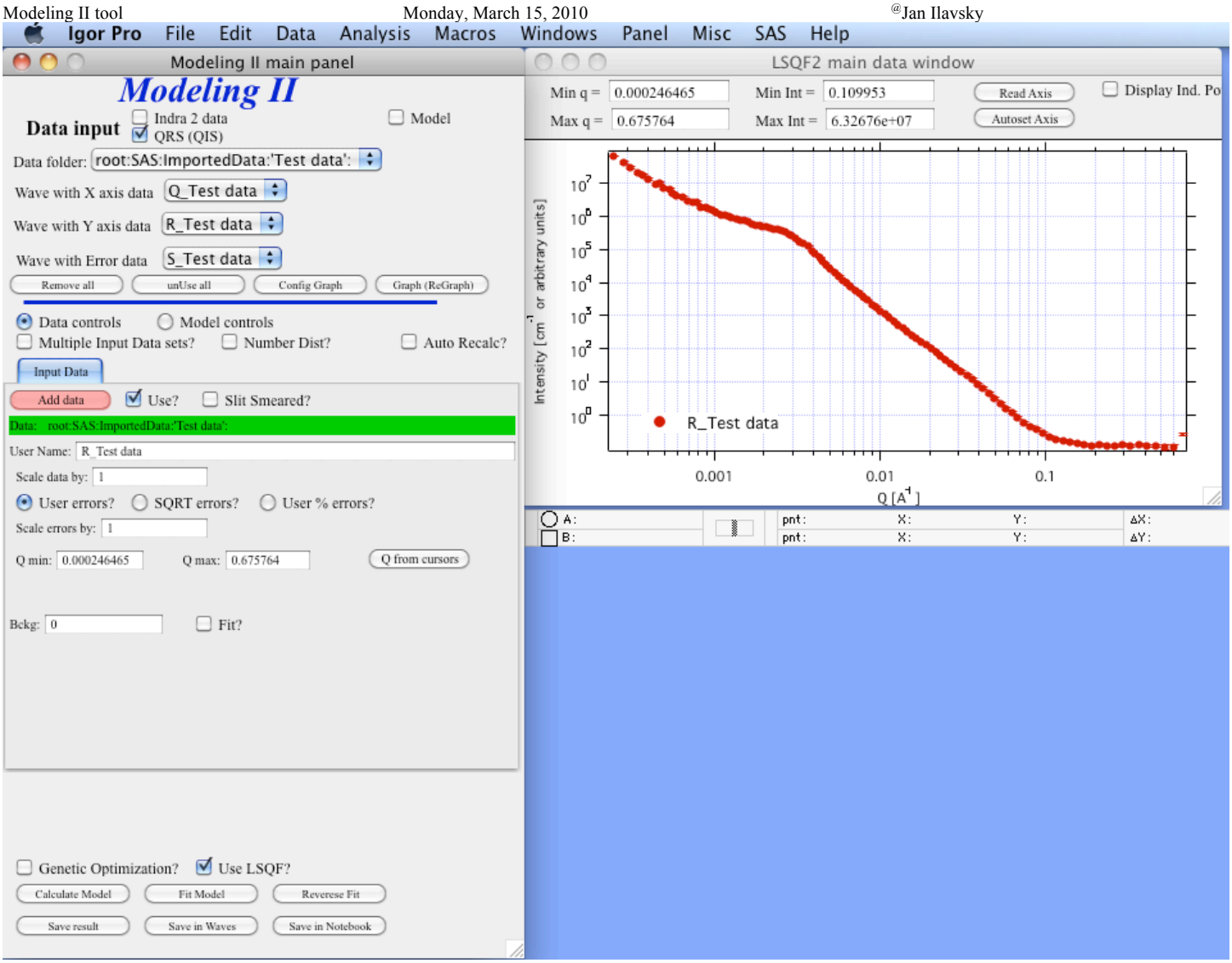
This panle is bit more complicated. At the top is usual Data selection set of controls. Below are two “radio-checkboxes” which can set the tabbed area below to either “Data controls” or “Model controls”.

Adding data in Modeling II

Keep “Data controls” selected.

By default the tools comes with only one input data set enabled. If you have multiple data sets for analysis, you would check the “Multiple Input data sets” checkbox – but for that read the manual.

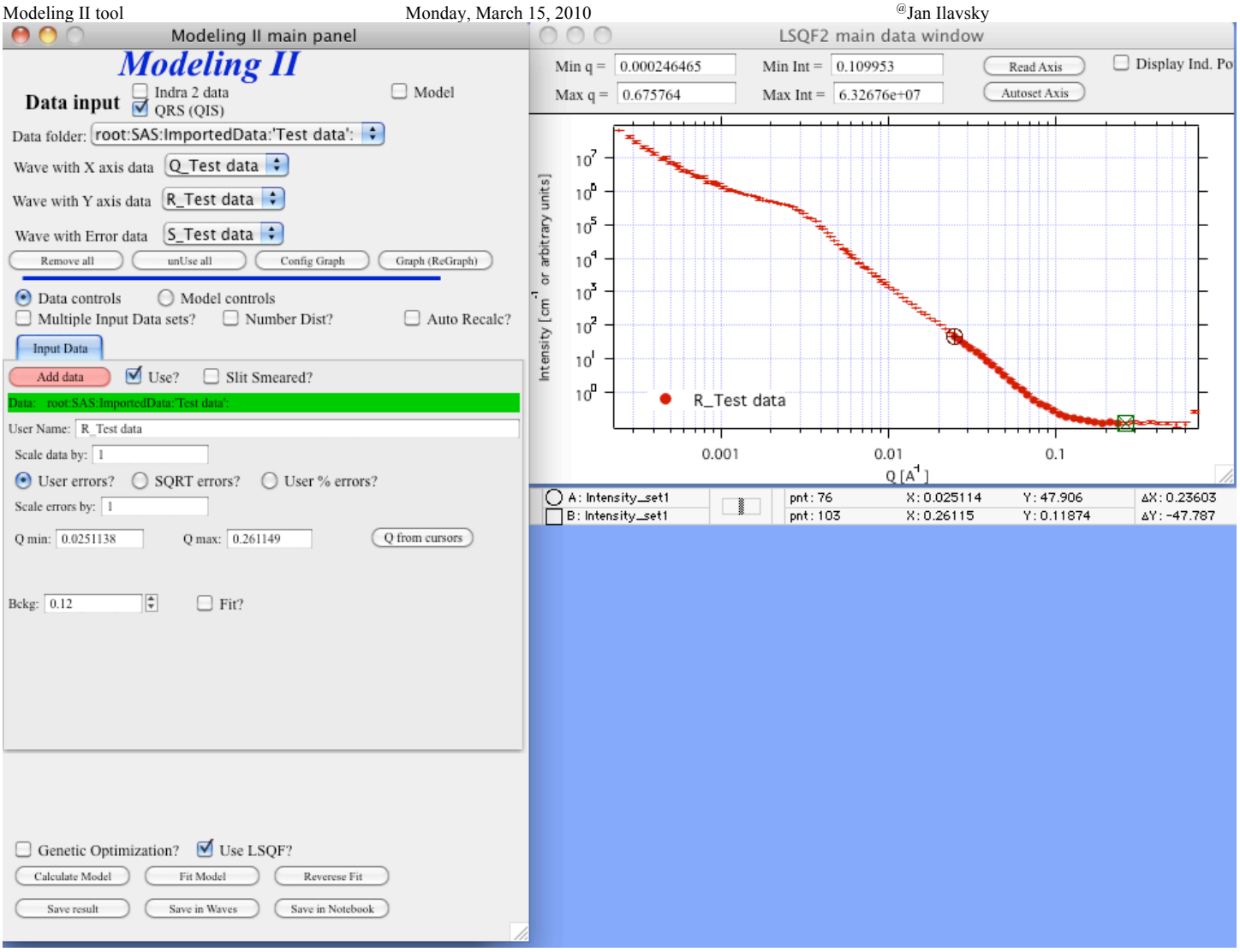
Select at the top part of panel the data you want to add. Select in our case “QRS (QIS)” checkbox and select the loaded data. Then push red button “Add data”:



Now the data are in. We need to set few other options at this moment…

Background. Flat background present in the data is subtracted here. Therefore we need to input estimate (to be refined later). 0.12 is a good number.

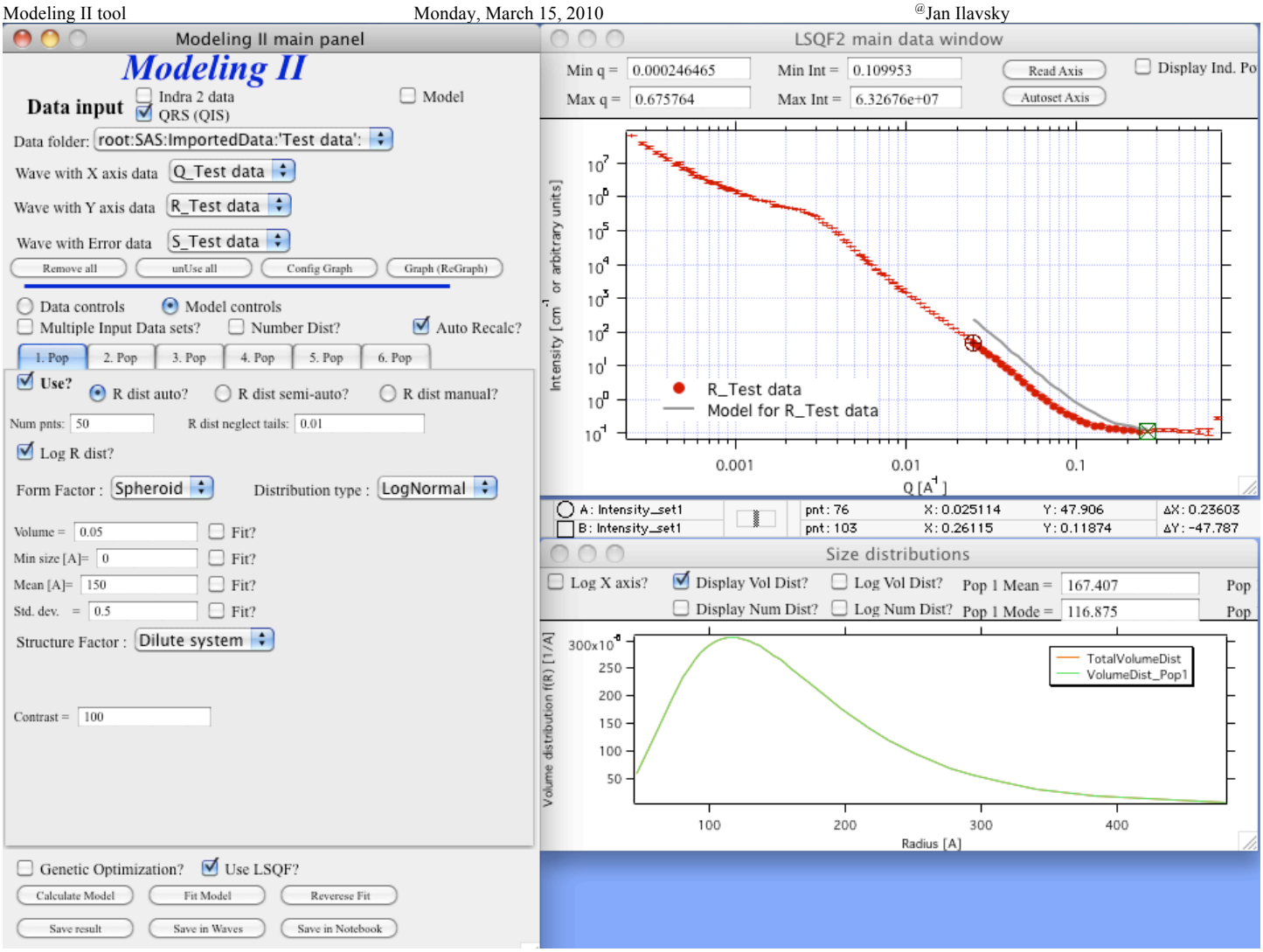
Data selection. We need to select range of data to be fitted with the model. We will use two populations of long-normal spheres to model the data. Let's start with the small particles and so we need to select first the high Q region – may be points from 76 to 103 or so. You can put cursors on the points and push button "Q from cursors".



Note, how the points changed. Only the circles will be used for fitting…

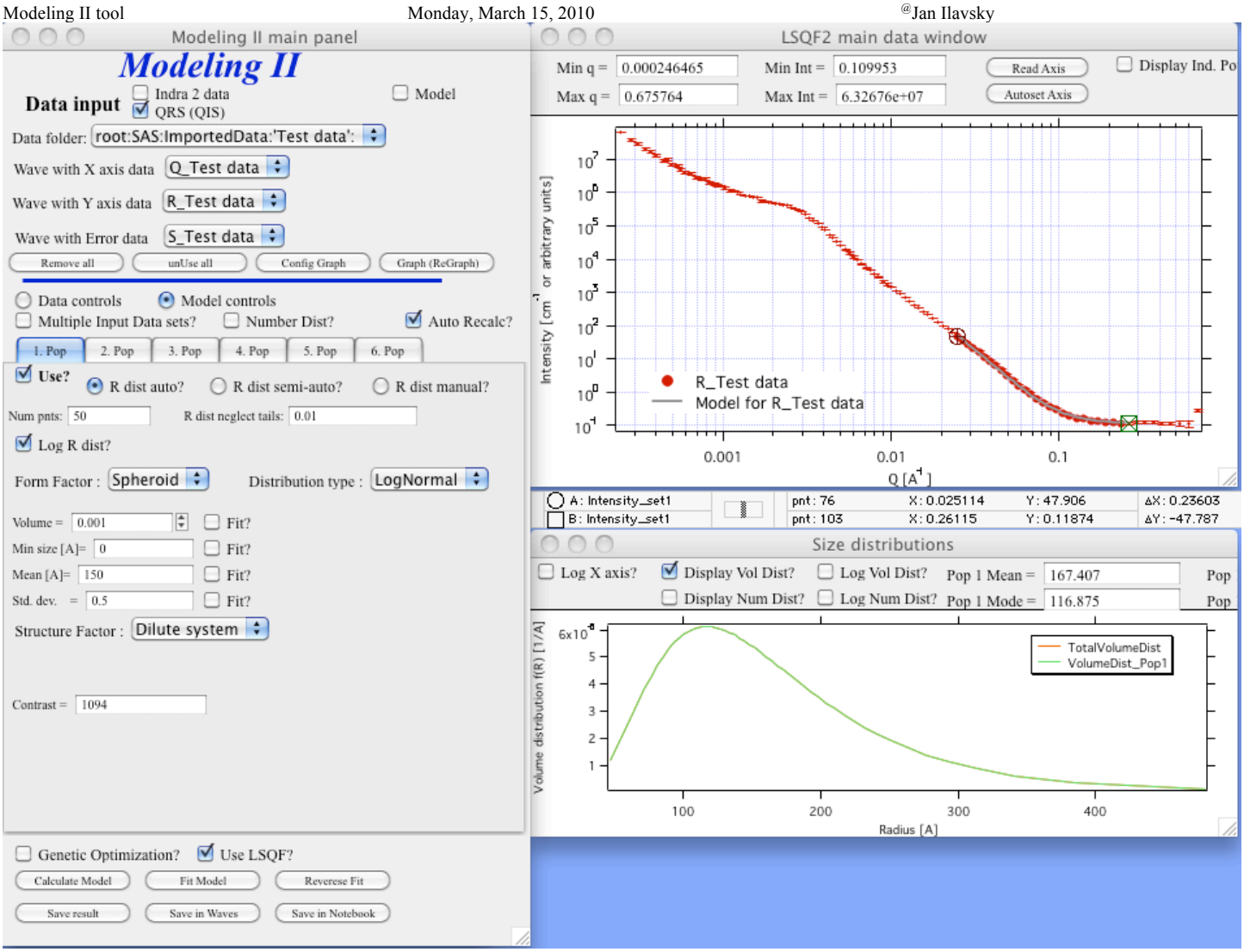
Model

Select “Model controls”. 6 populations are now available to you. You can use any (and all) populations. Lets use 1 Pop. Click checkbox “Use?” and control appear. Also for simplicity, select “Auto recalc?” checkbox. This causes code to recalculate model every time you make any change.



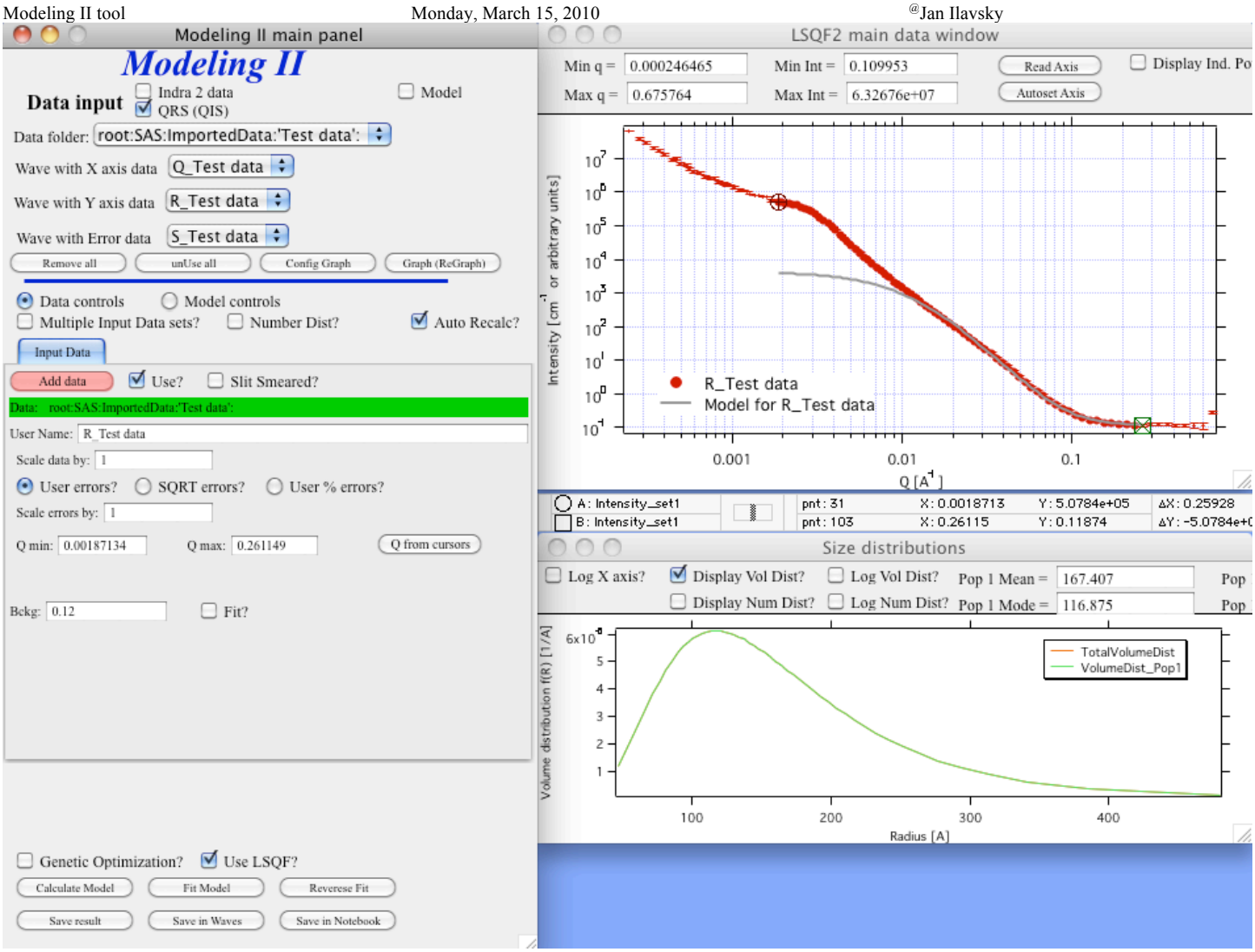
The grey curve in the graph is the calculated intensity from the model. Let's modify some parameters here.

Contrast fro alumina is 1094 (even though these data are not calibrated). The mean diameter is about 170A for the default parameters, which is reasonably close to the evaluation from Size distribution. Just reduce the volume to 0.001 to accommodate the change in cotrast and the curve should be reasonably well estimated:



Next we need to evaluate the large features, which are about 1500A large (running Size distribution first helps ☺).

First let's increase the range of data analyzed here. Go to "Data controls again, use cursors to select range of data from point about 31 to 103 and push button "Q from cursors". In this case the code does not recalculate automatically, so you can force calculation using button "Calculate model".
This is the estimate with just these fine particles:



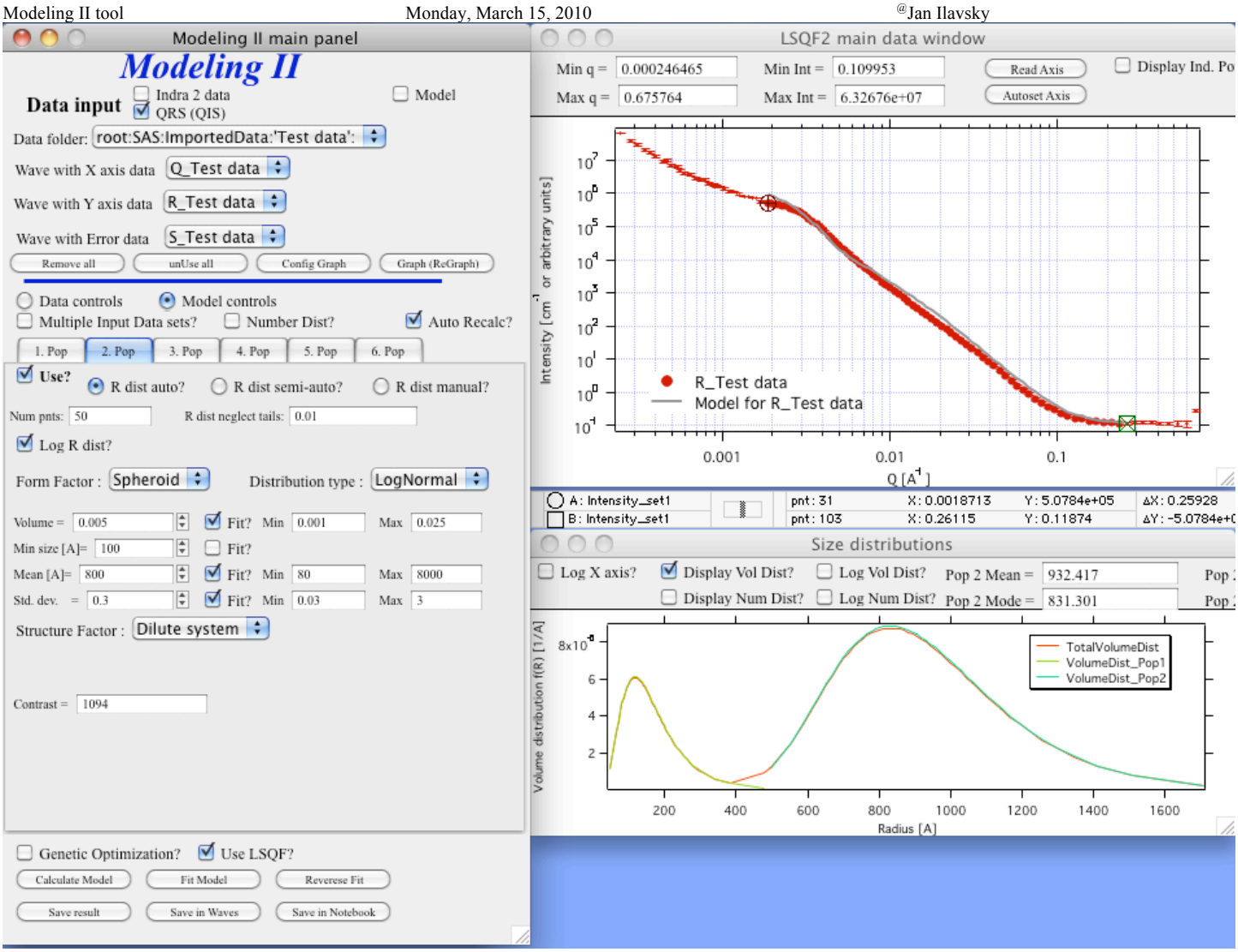
Let's got back to "Model controls", select "2. Pop" and click on checkbox "Use?"

Next we need to estimate the values for the log-normal size distribution. Contrary to Gaussian this one is really not intuitive. I usually play with the parameters until I get in the distribution graph something sensible and then do fitting.

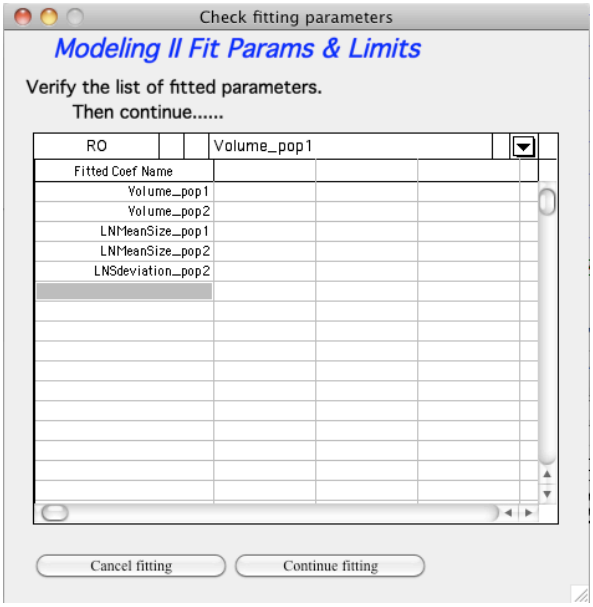
My wild guess is: Contrast 1094, Volume 0.005, min size 100, Mean 800, Std. dev. 0.3. This produces something, which may fit…

Select For "1. Pop" following Fit? checkboxes:
Volume and Mean

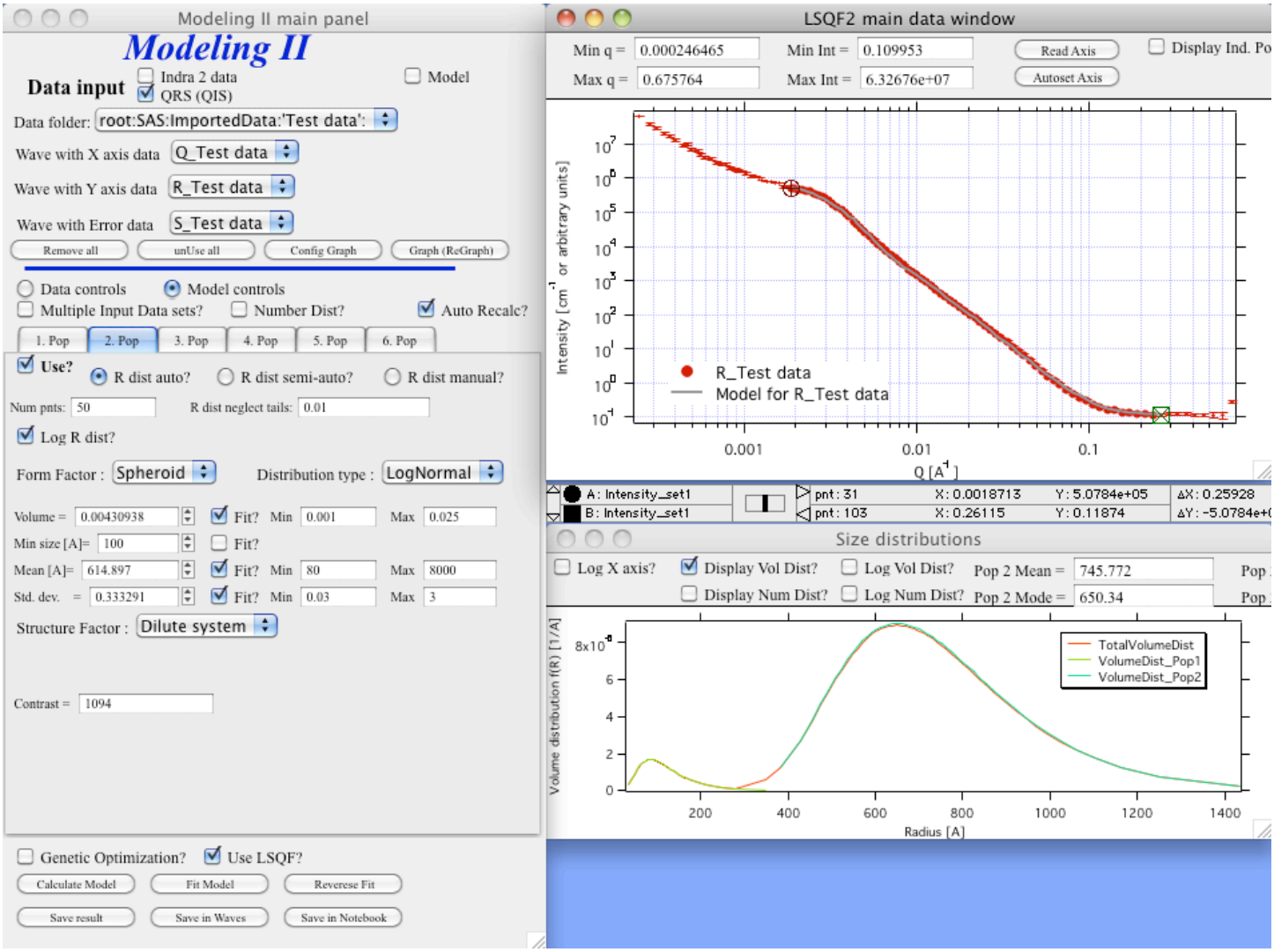
Select for "2. Pop" following checkboxes:
Volume, Mean, Std dev.



Push button “Fit”. You get another panel with list of parameters selected for fitting. This panel is here mainly for use of Genetic optimization (note: that methods takes long time to iterate, but can be superior in results. Before using make sure you read the manual).



This list tells you which parameters (using internal parameter names) are fitted. Say "Continue" and you will get fit:



Now we can select more checkboxes for fitting and fit more parameters. Fitting of background is controlled on "Data controls screen".

Note, that fitting of "Min size" is usually not very sensitive for these distributions.

You can now save results in the folder for future use (and comparison for example with Size distribution etc.), you can save waves with results (read manual for meaning) or save in notebook, which produces following record. This record contains probably all information you ever wanted to know.

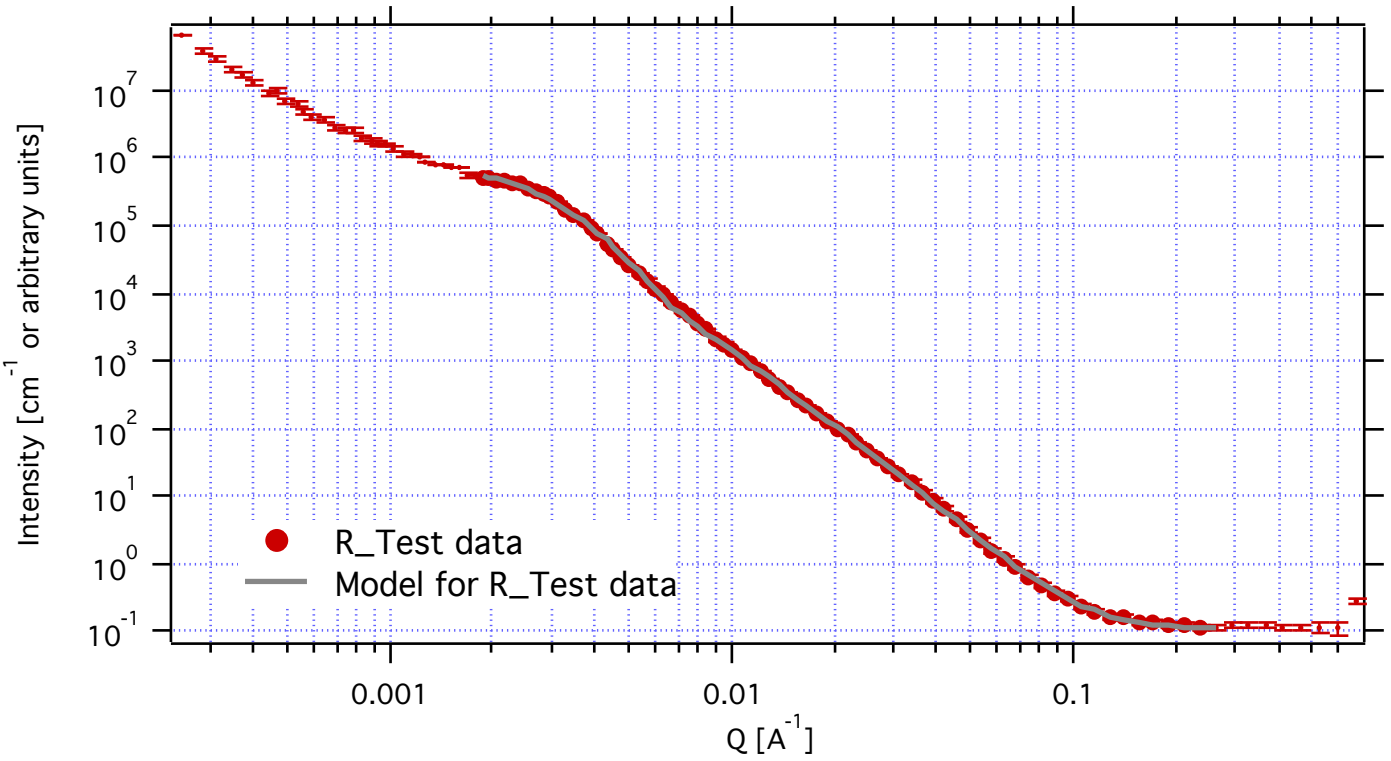
This is output of results from Modeling II of Irena package.

3/22/10, 3:49 PM
****

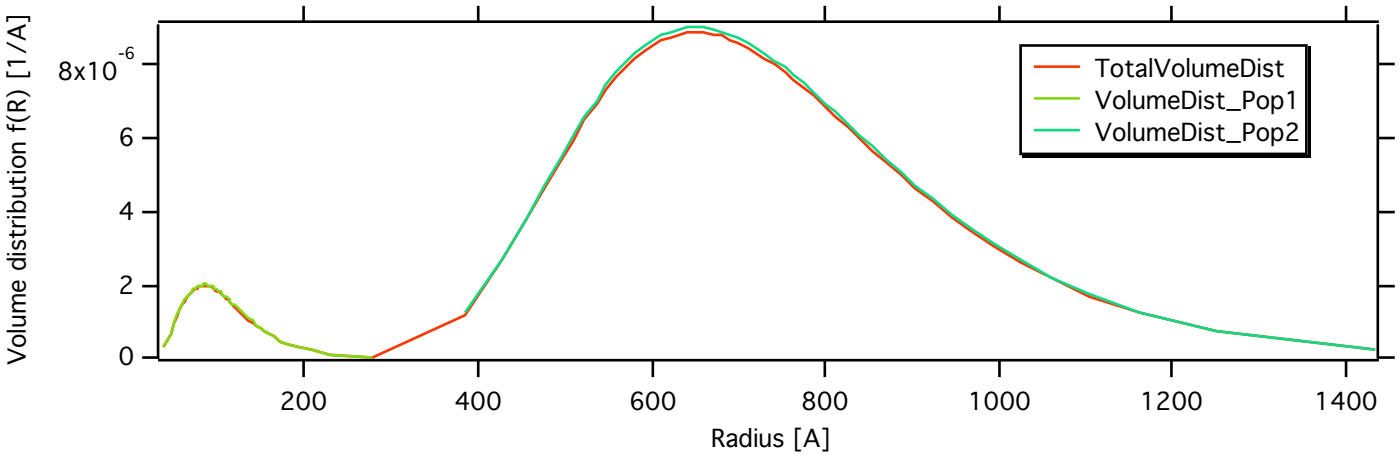
Results saved on Mon, Mar 22, 2010 3:49:35 PM

Single data set used:
FolderName_set1 = root:SAS:ImportedData:'Test data':
IntensityDataName_set1 = R_Test data
QvecDataName_set1 = Q_Test data
ErrorDataName_set1 = S_Test data
UserDataSetName_set1 = R_Test data
DataScalingFactor_set1 = 1
ErrorScalingFactor_set1 = 1
Qmin_set1 = 0.0018713
Qmax_set1 = 0.26115
Background_set1 = 0.10739

LSQF2 main data window



Size distributions



Model data for 2 population(s) used to obtain above results

Summary results for 1 population
Volume_pop1 = 0.0002
Mean_pop1 = 110.35
Mode_pop1 = 84.359
Median_pop1 = 101.8
FWHM_pop1 = 89.583

Distribution type for 1 population
DistributionShape_pop1 = Gauss
GaussMean_pop1 = 150
GaussWidth_pop1 = 50

Contrasts for data set 1 population
Contrast_pop1=1094

Form factor description and parameters
FormFactor_pop1 = Spheroid
Aspect Ratio FormFactor_Param1_pop1 = 1

Structure factor description and parameters
StructureFactor_pop1 = Dilute system

Summary results for 2 population
Volume_pop2 = 0.0043133
Mean_pop2 = 746
Mode_pop2 = 650.88
Median_pop2 = 715.81
FWHM_pop2 = 442.68

Distribution type for 2 population
DistributionShape_pop2 = Gauss
GaussMean_pop2 = 300
GaussWidth_pop2 = 100

Contrasts for data set 2 population
Contrast_pop2=1094

Form factor description and parameters
FormFactor_pop2 = Spheroid
Aspect Ratio FormFactor_Param1_pop2 = 1

Structure factor description and parameters
StructureFactor_pop2 = Dilute system

Conclusions

Modeling II enables you to model data with up to 6 populations to scatterers – each population is independent, can have separate Form factor, structure factor, shape and contrast. Up to 10 input data sets can be fitted at the same time.

You can fit data measured using different wavelengths (using different contrasts for each data set-population combination), measured on X-rays and neutrons, etc.